

1003149 101901

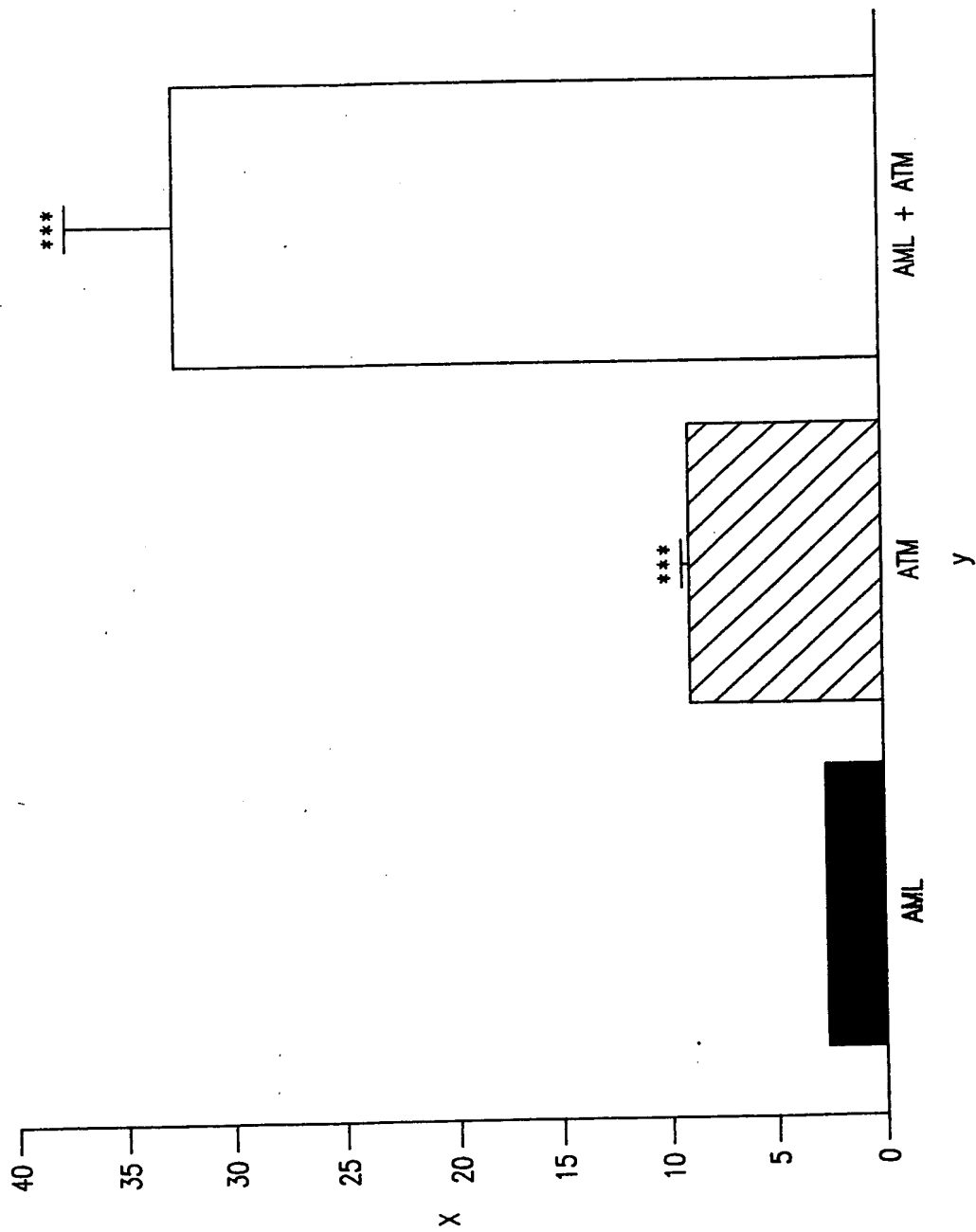


FIG. 1

TOGETHER EFFECT

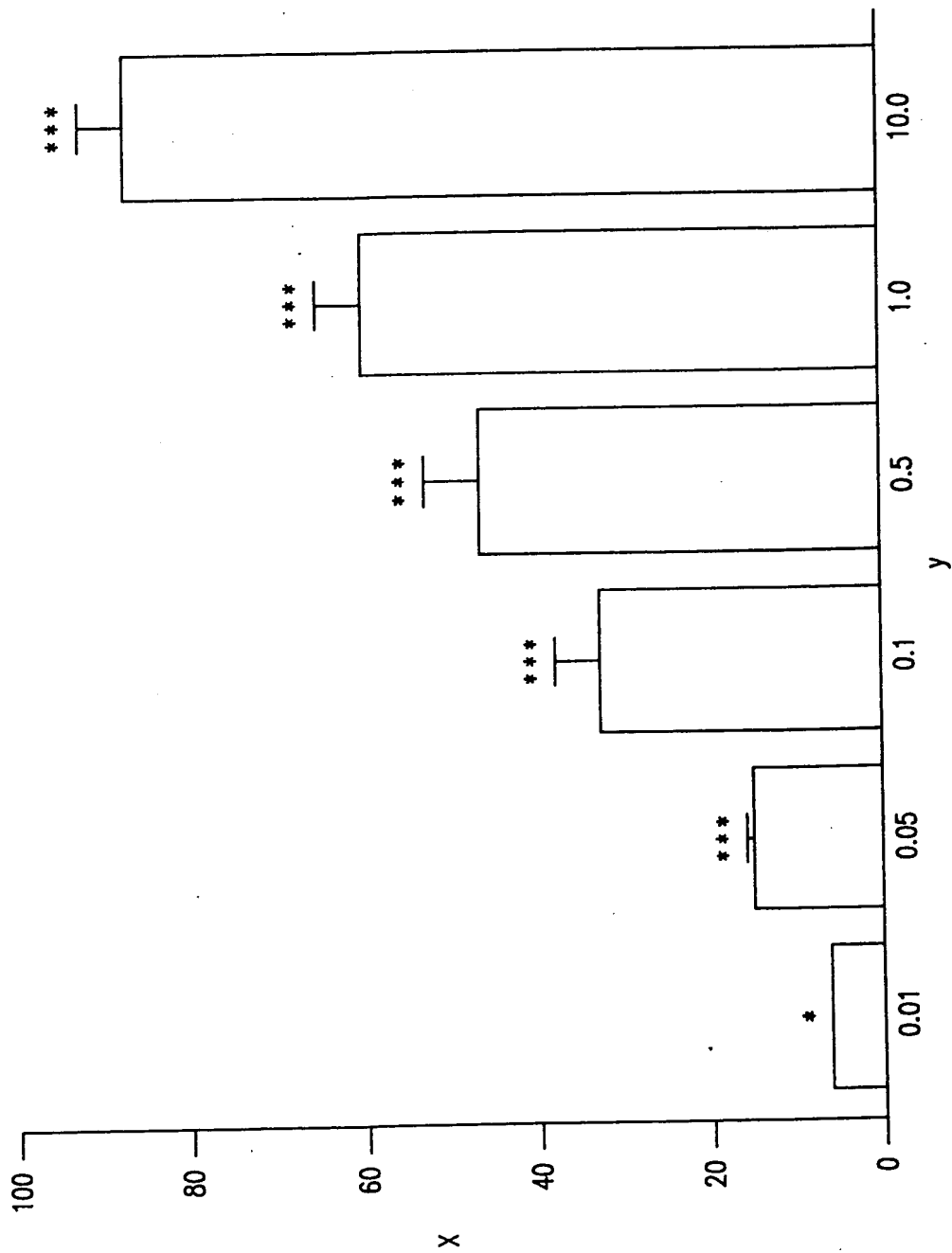


FIG. 2

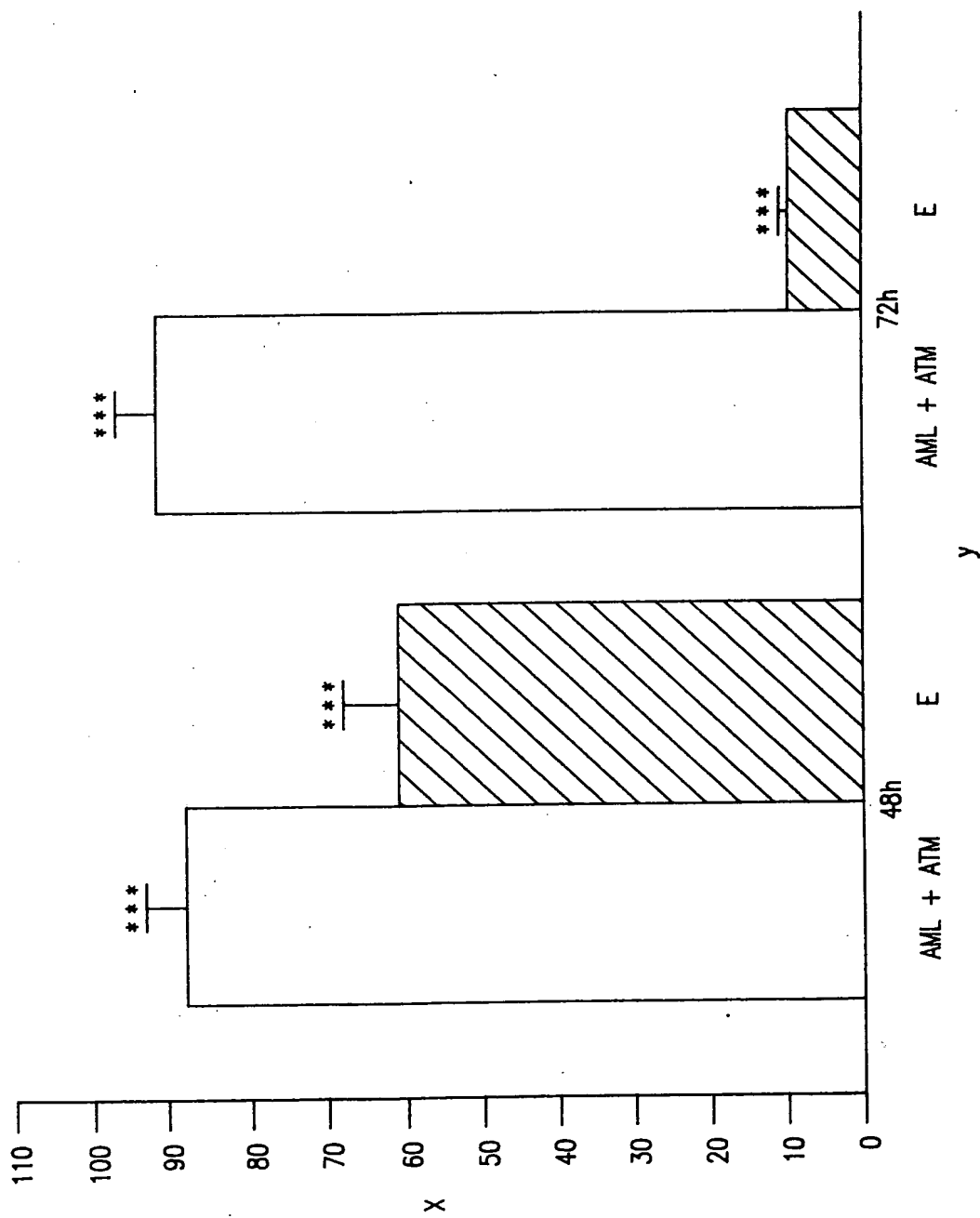
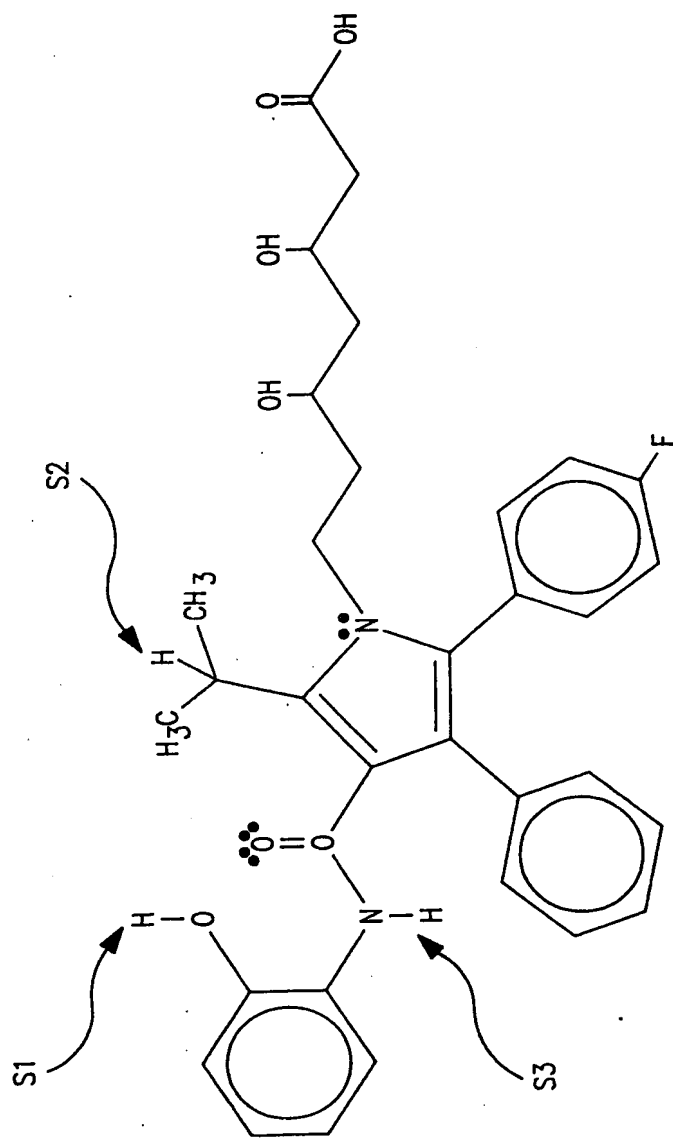


FIG. 3



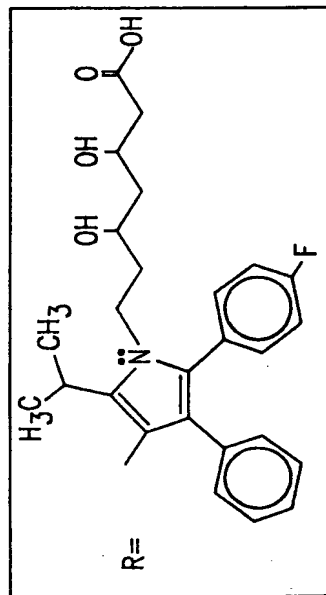
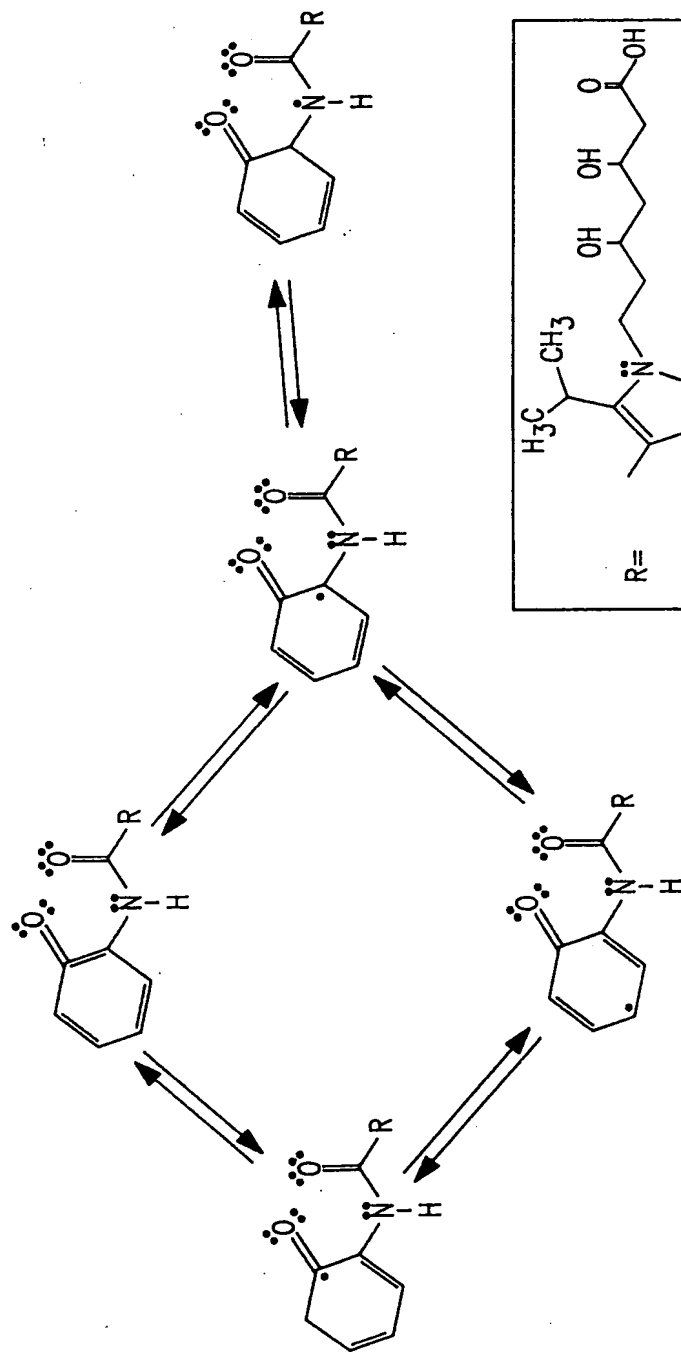


FIG. 4B

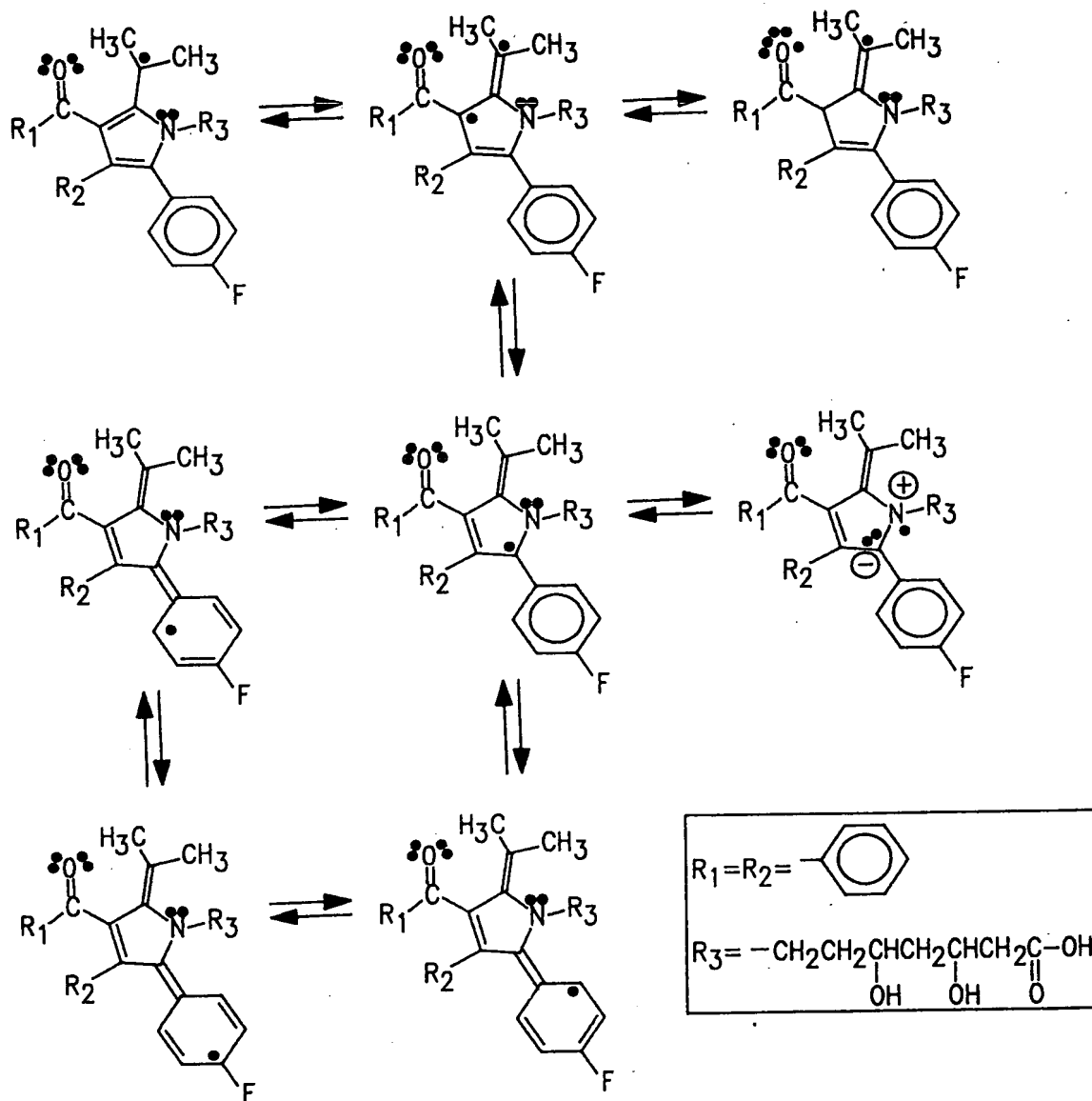


FIG. 4C

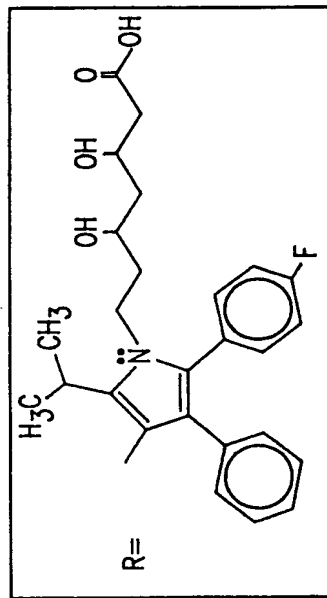
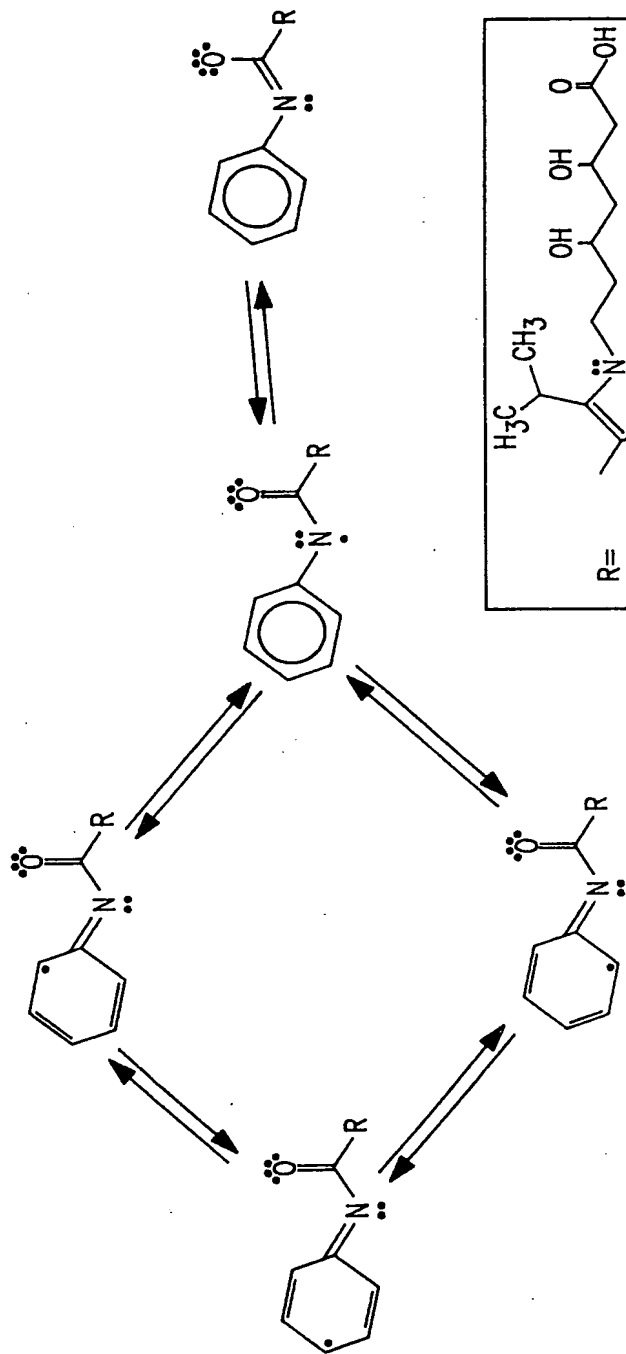


FIG. 4D

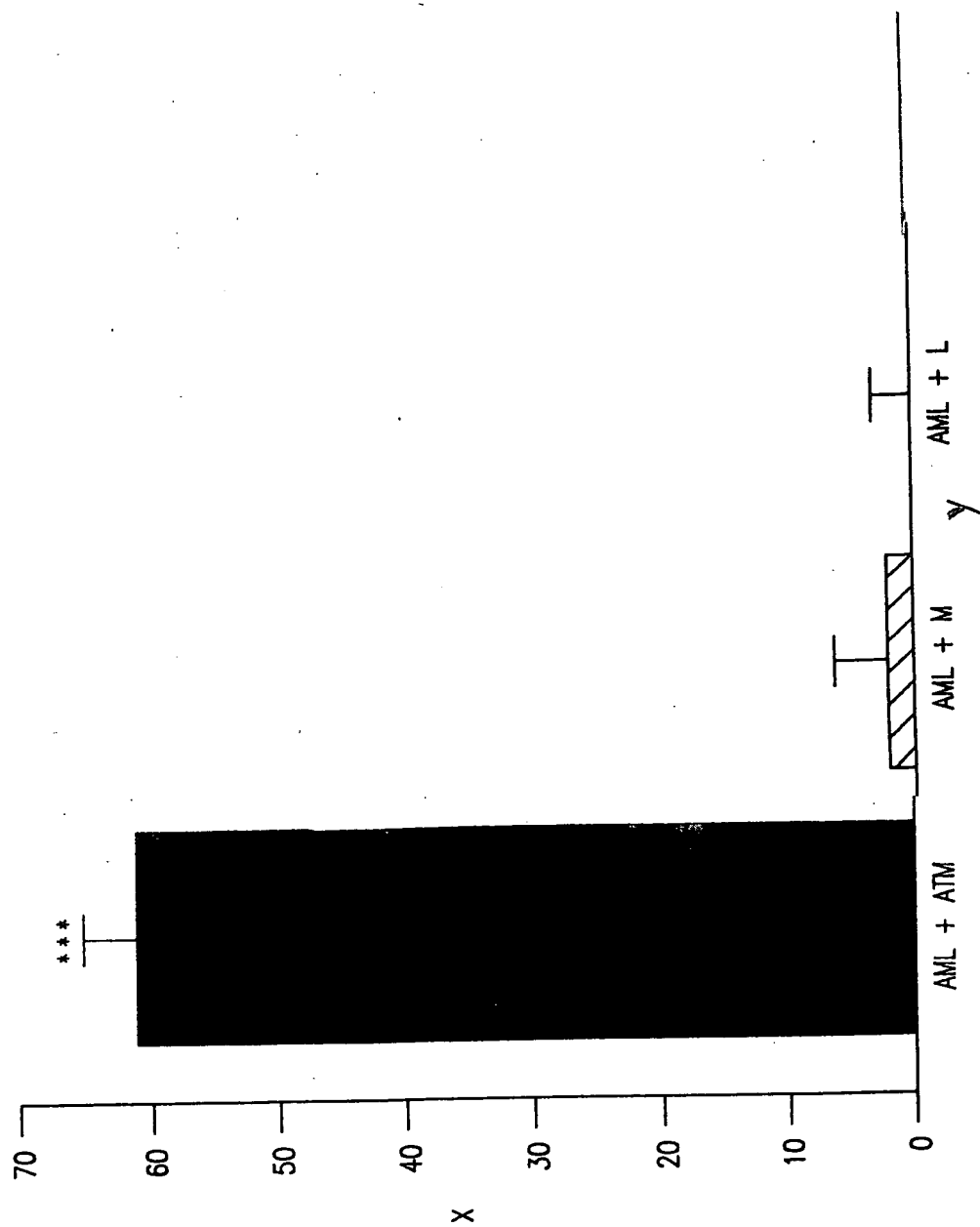


FIG. 5

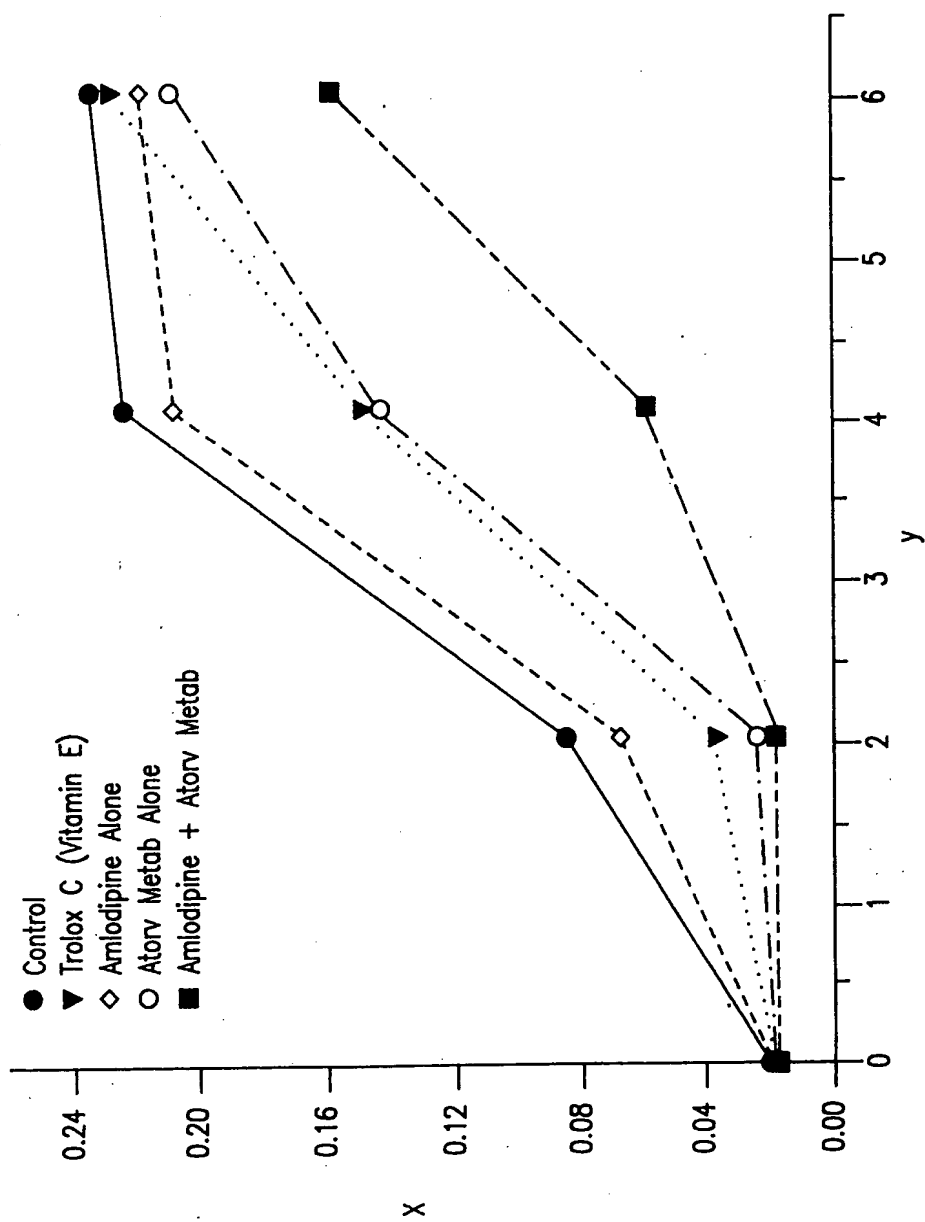


FIG. 6A

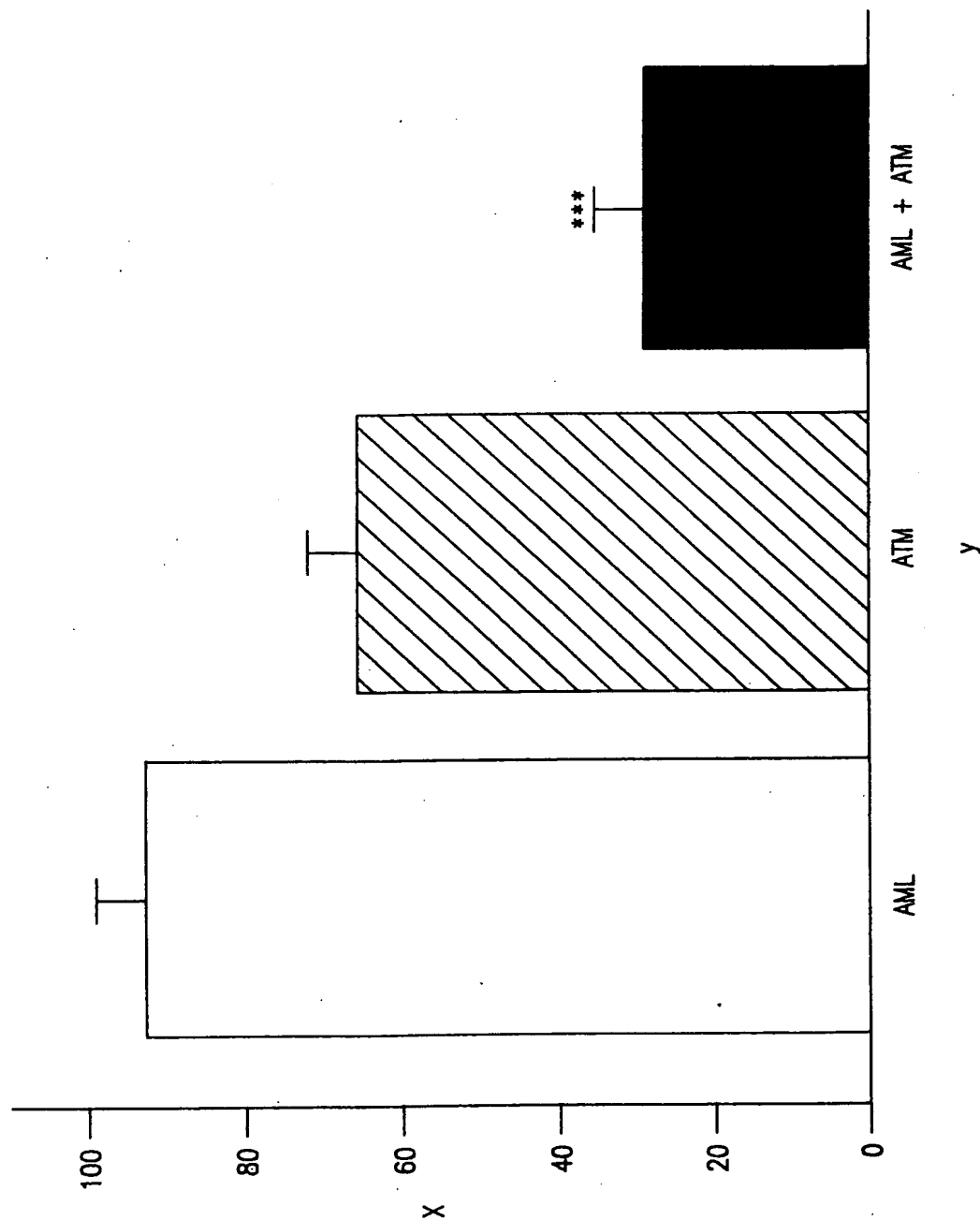


FIG. 6B

Computed Enthalpies of Formation for
Atorvastatin Metabolite Radicals *

Molecule	ΔH_f (kcal/mol)
Carbon radical	-209.50
Oxygen radical	-199.89
Nitrogen radical	-192.55
Methyl radical	-193.51
Phenyl radical	-176.05
Carbon/Oxygen Diradical	-182.07
Carbon/Nitrogen Diradical	-174.25

*The smaller (i.e., more negative) the ΔH_f value, the easier to abstract the H atom from that site.

Computed Enthalpies of Formation for
Amlodipine Radicals *

Molecule	ΔH_f (kcal/mol)
Carbon radical	-164.28
Nitrogen radical	-148.27

*The smaller (i.e., more negative) the ΔH_f value, the easier to abstract the H atom from that site.

FIG. 7

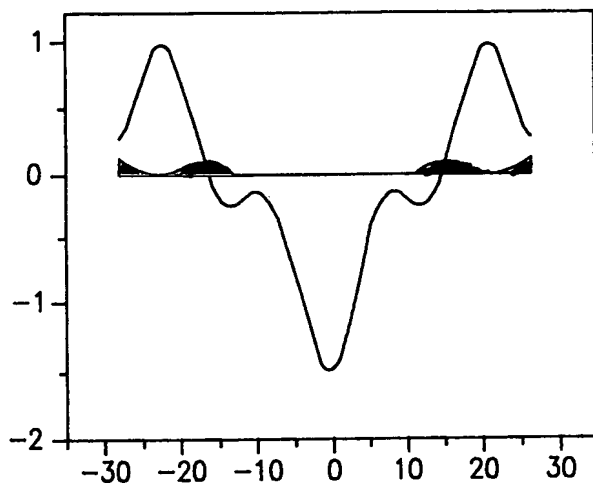


FIG. 8A

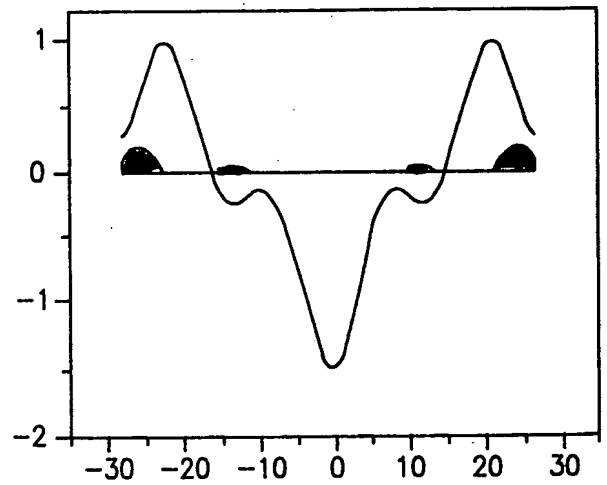


FIG. 8B

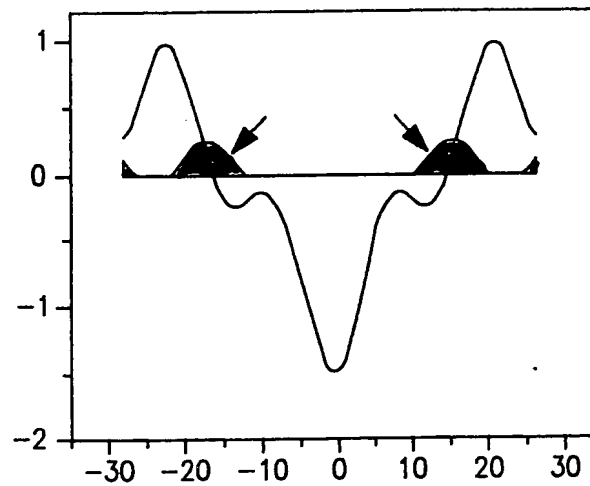


FIG. 8C

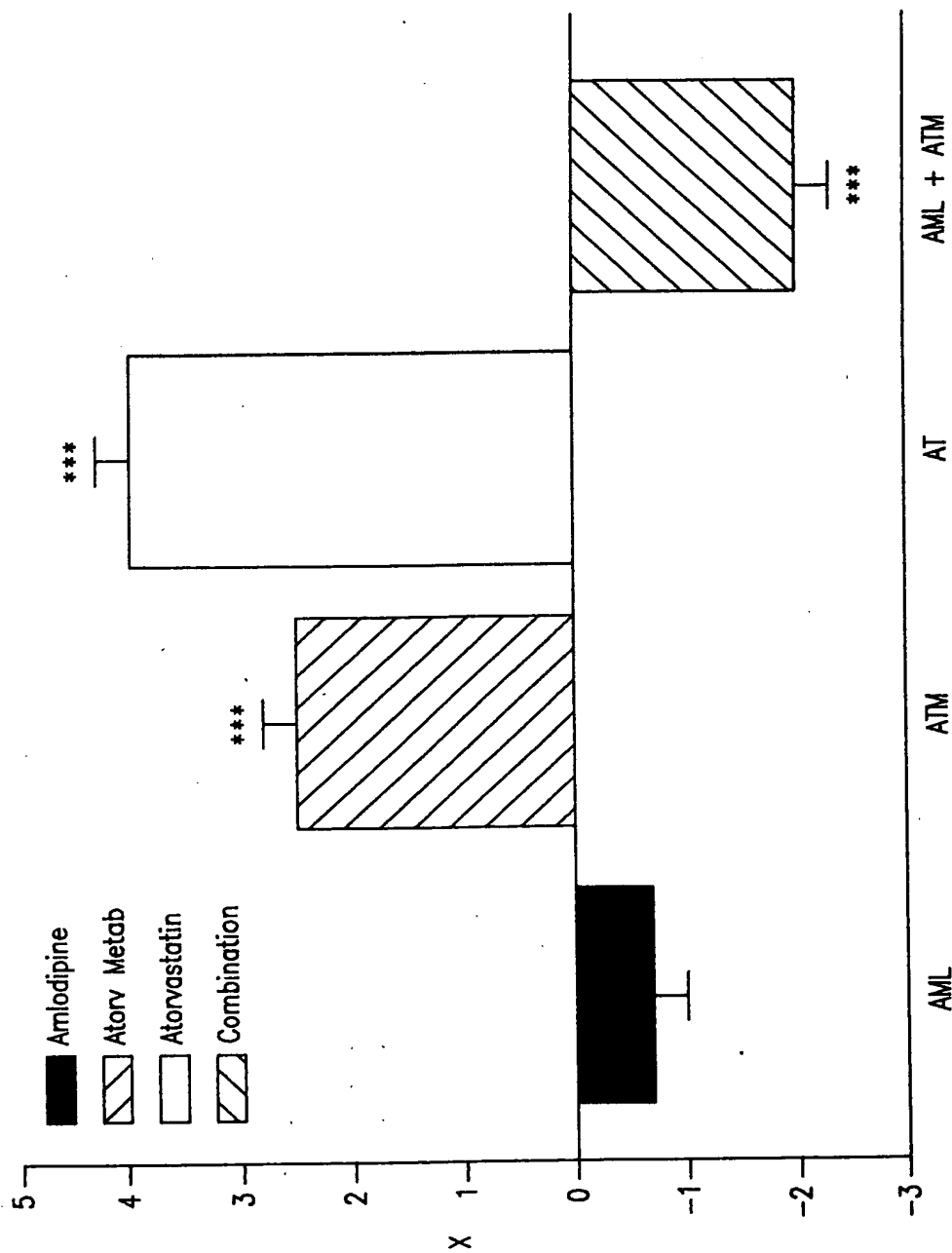


FIG. 9